

h-mmp8
h-mmp3
h-mmp1

210	220	230	240
LAHSSDPGALMYPNY - AFRETSNYSLP	QDDIDG IQAIYG		
LFHSANT EALMYPPLYHSLTDLTRFRLS	QDDINGI QSLYG		
LSHSTDIGALMYP SY - TF - -SGDVQLA	QDDIDG IQAIYG		
* * *	* * *	* * *	* *

Figure 2

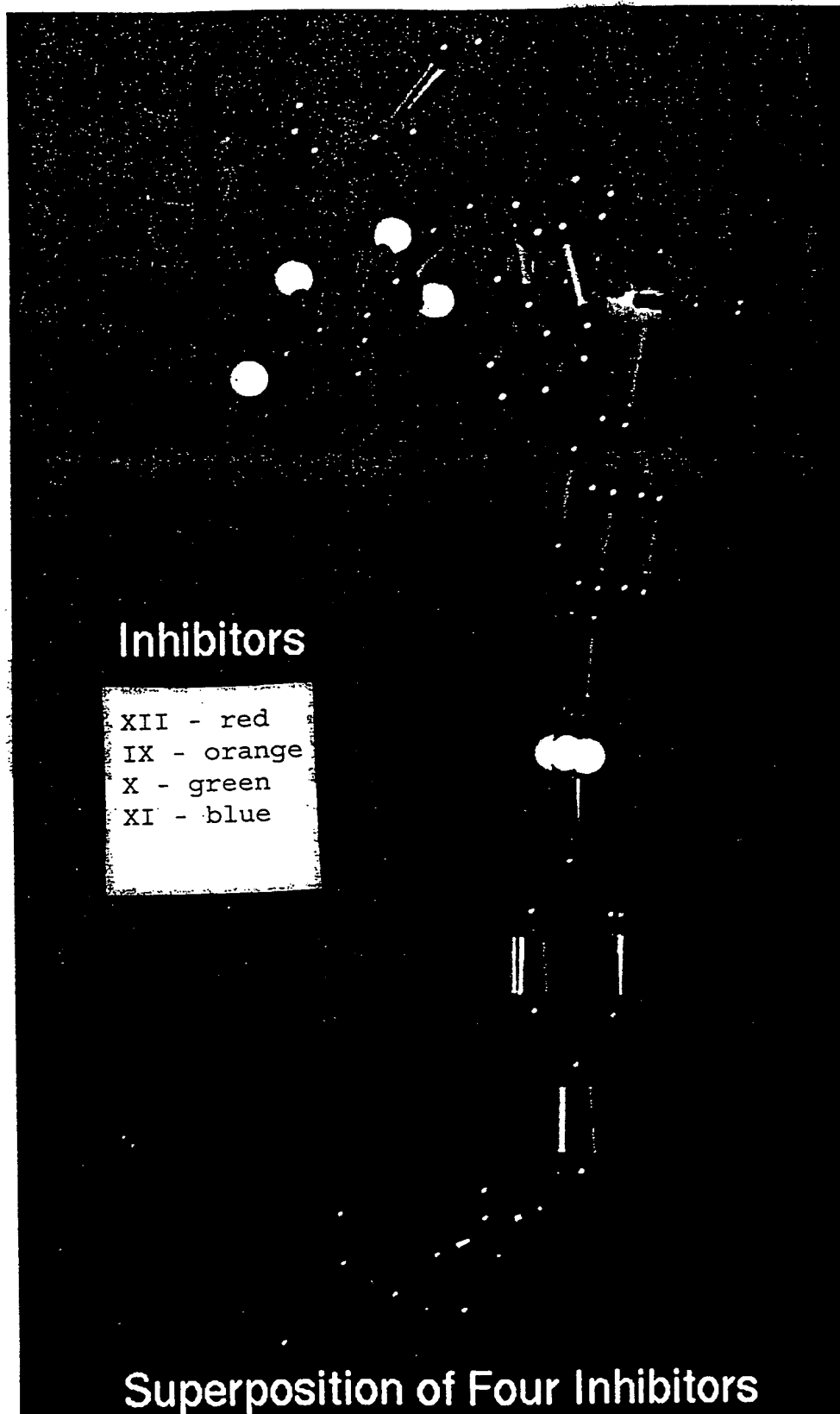


Figure 3

Interacting Residues Within 5 A of the Inhibitor Molecule						
		XII	IX	X	XI	XIV
L119	no					no
G158						
I159						
L160						
A161						
H162						
A163	no					
L193						
V194						
A196	no	no			no	no
H197						
E198						
H201						
H207						
G212		no	no			no
A213						
L214						
Y216						
P217						
N218						
Y219						
A220						
R222						
T224	no					no
Y227		no	no	no	no	no
S228	no					no
P230						no

Figure 4

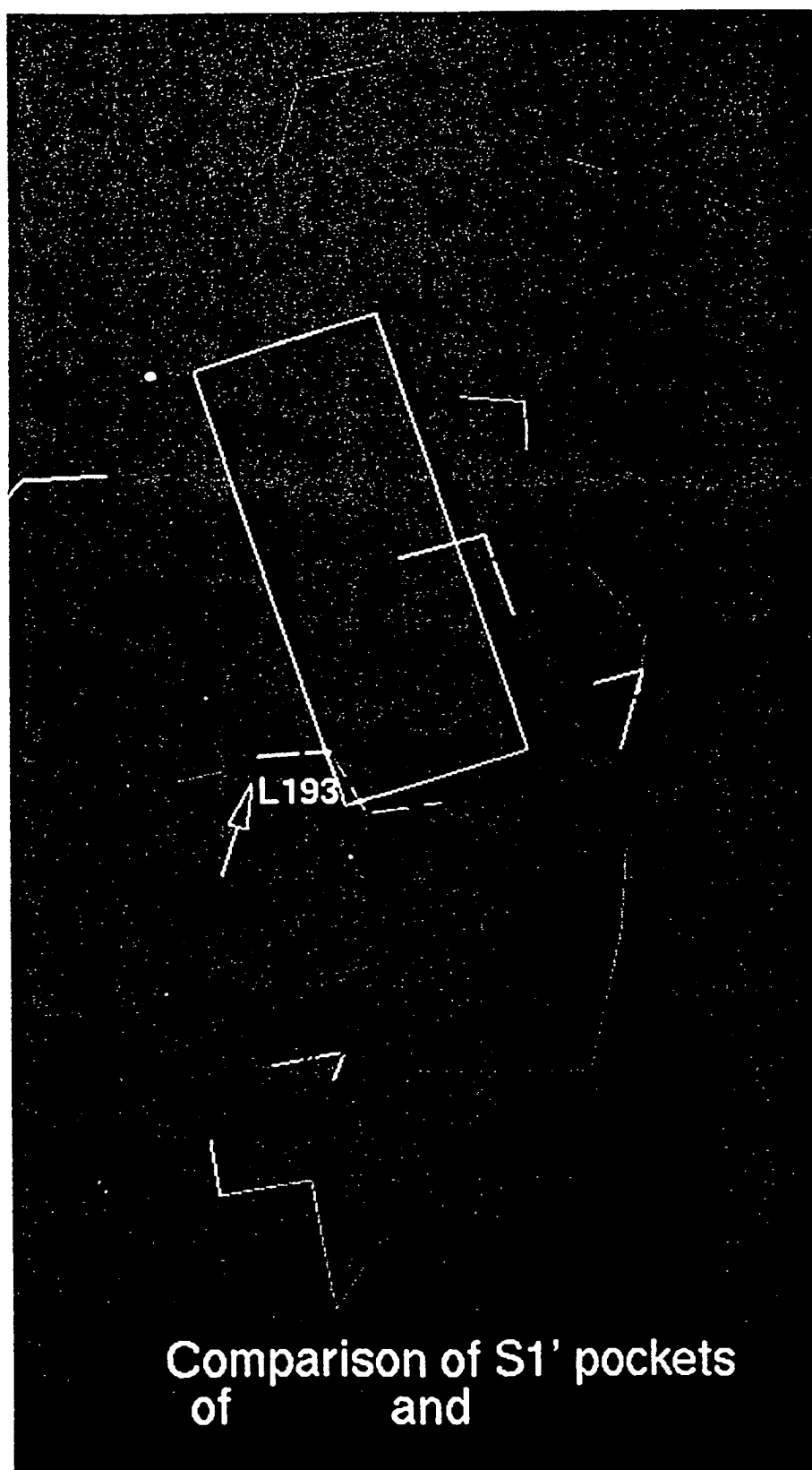


Figure 5

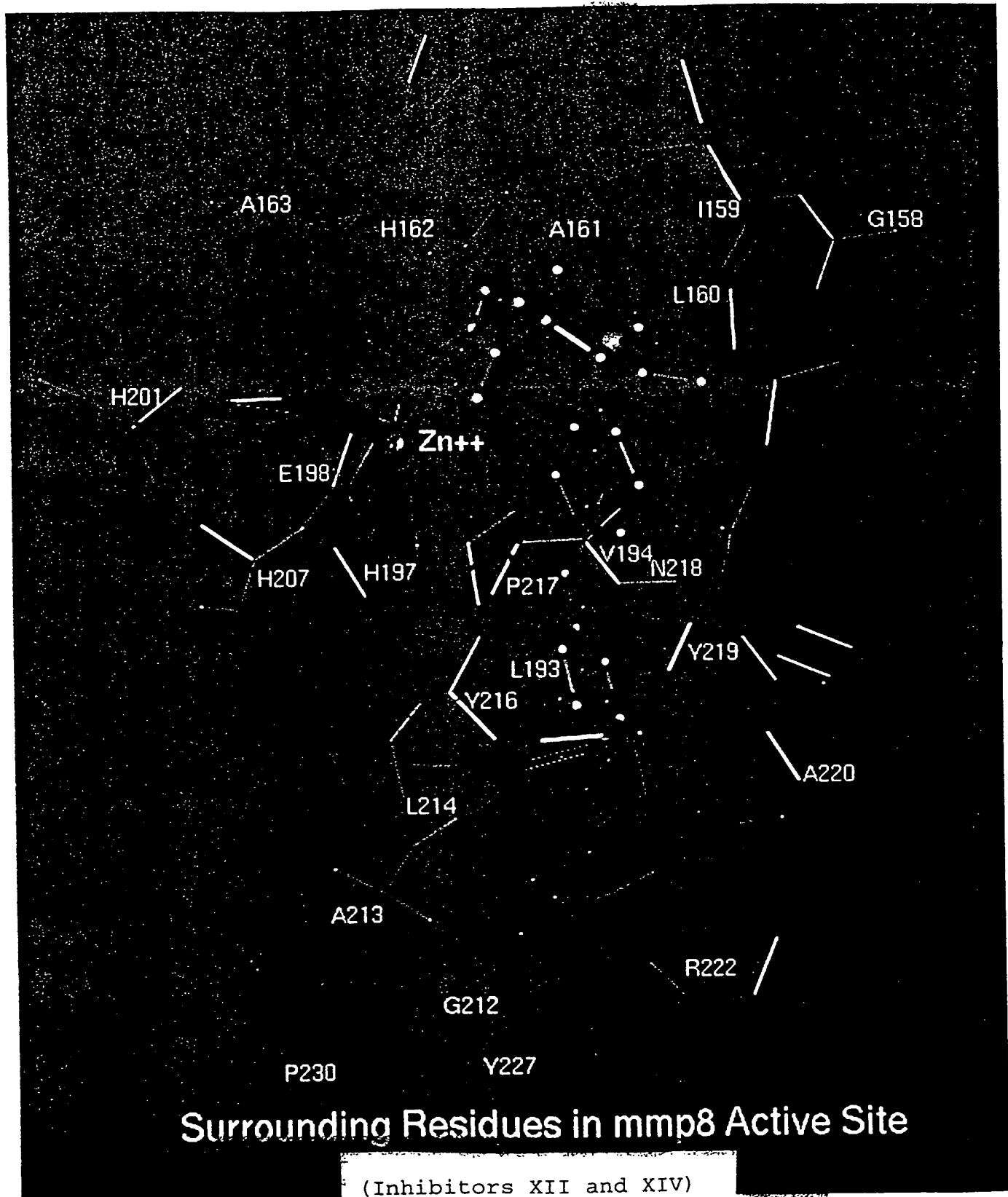
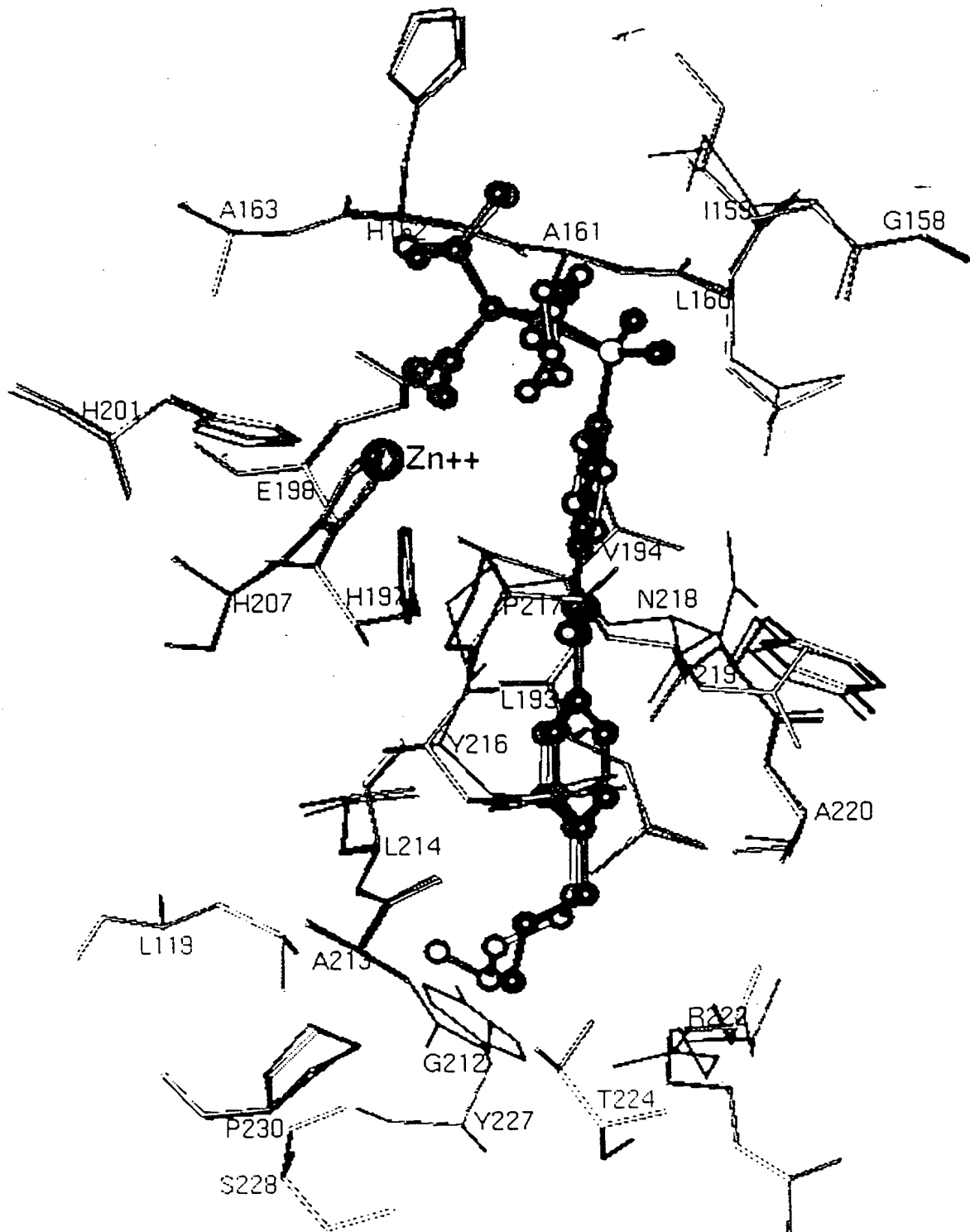
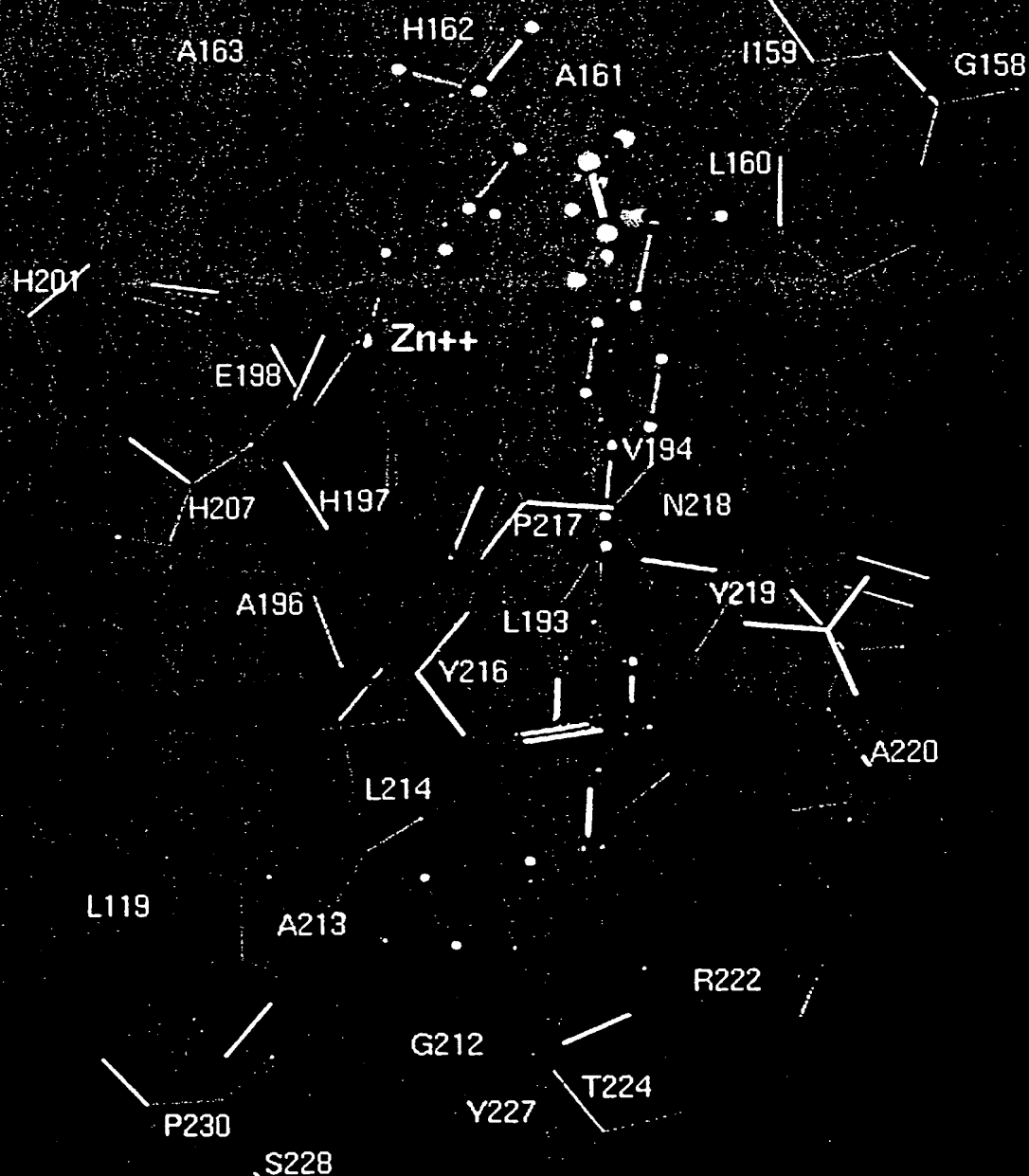


Figure 6



Surrounding Residues in mmp8 Active Site
(Inhibitors XII and IX)



Surrounding Residues in mmp8 Active Site

(Inhibitors XII and X)

Figure 8

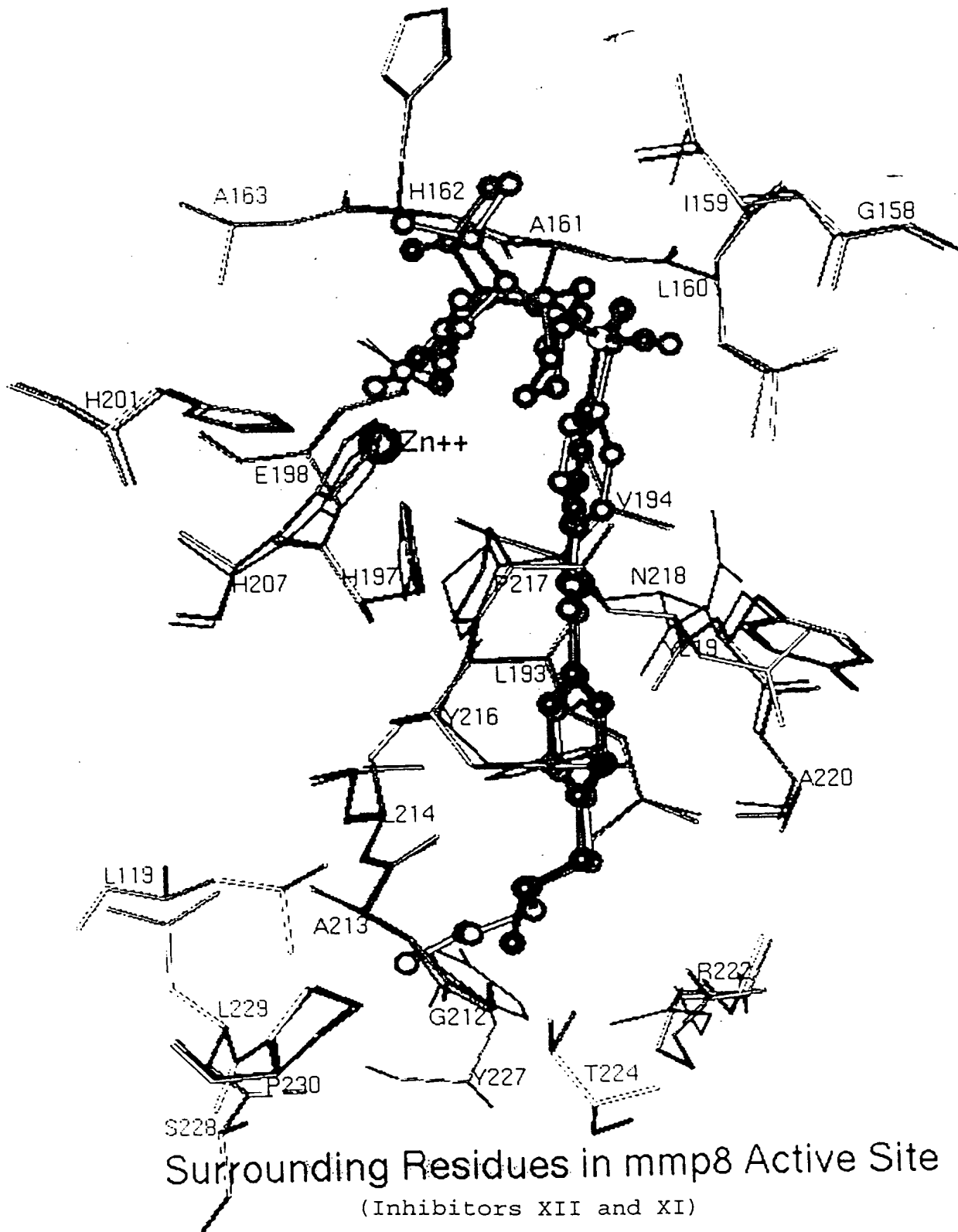


Figure 9

H207

P217

N218

Y216

P211

D210

Y227

R222

Inhibitor XIV (red)
Inhibitor XII (green)

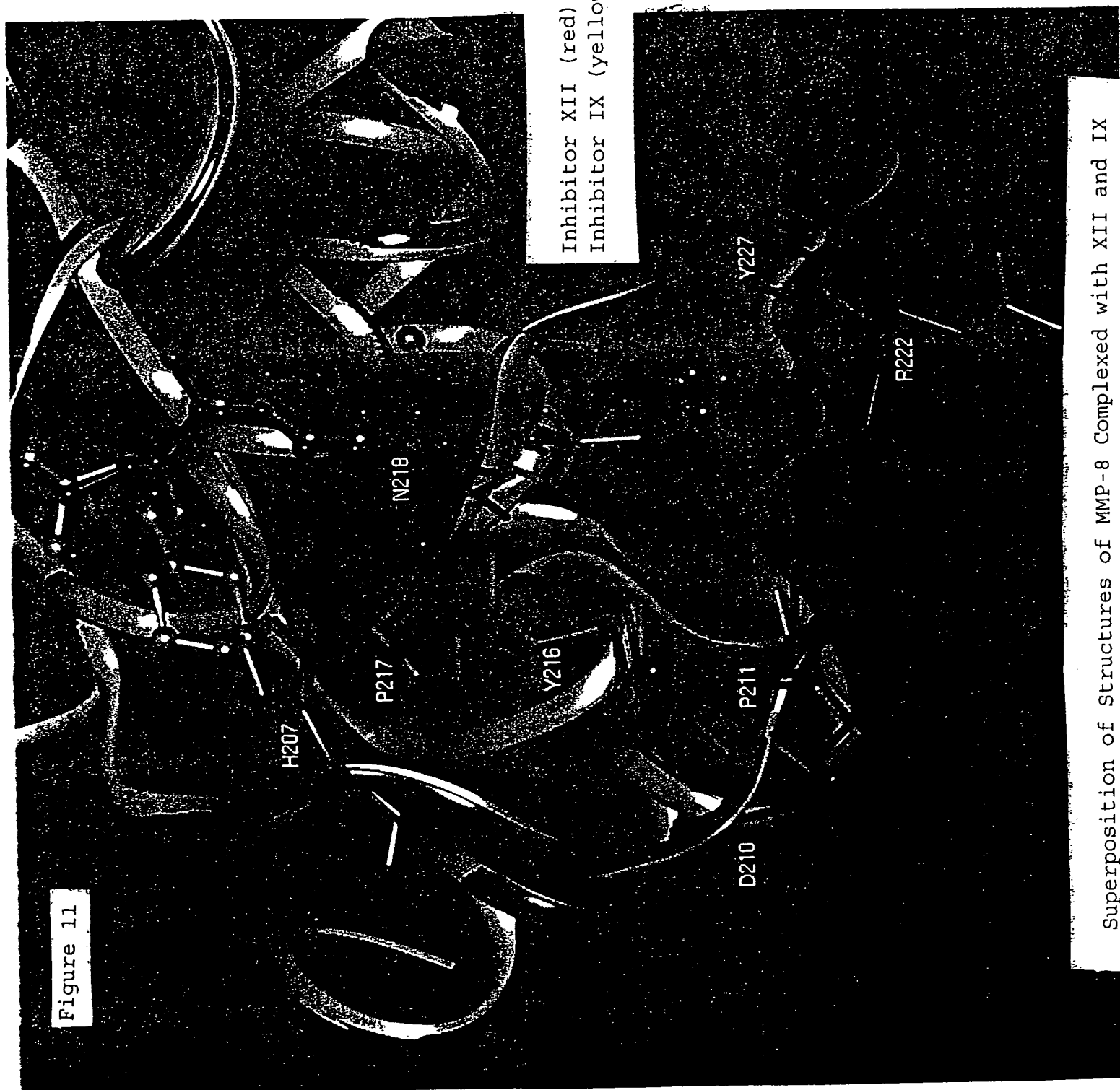
Superposition of Structures of MMP-8 Complexed with XII and XIV



Figure 10

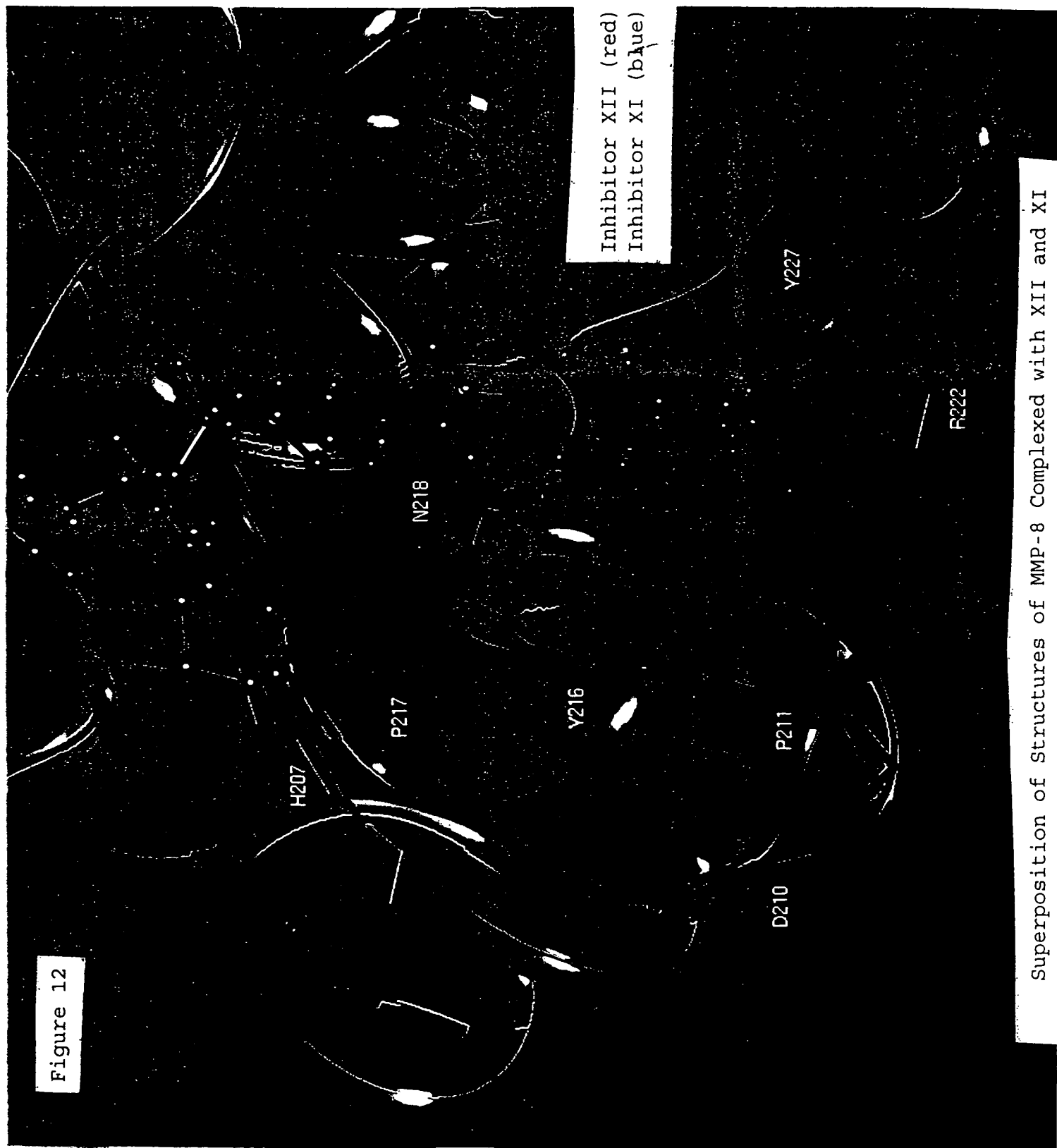
Superposition of structures of MMP-8 Complexed with XII and X

Figure 11



Superposition of Structures of MMP-8 Complexed with XII and IX

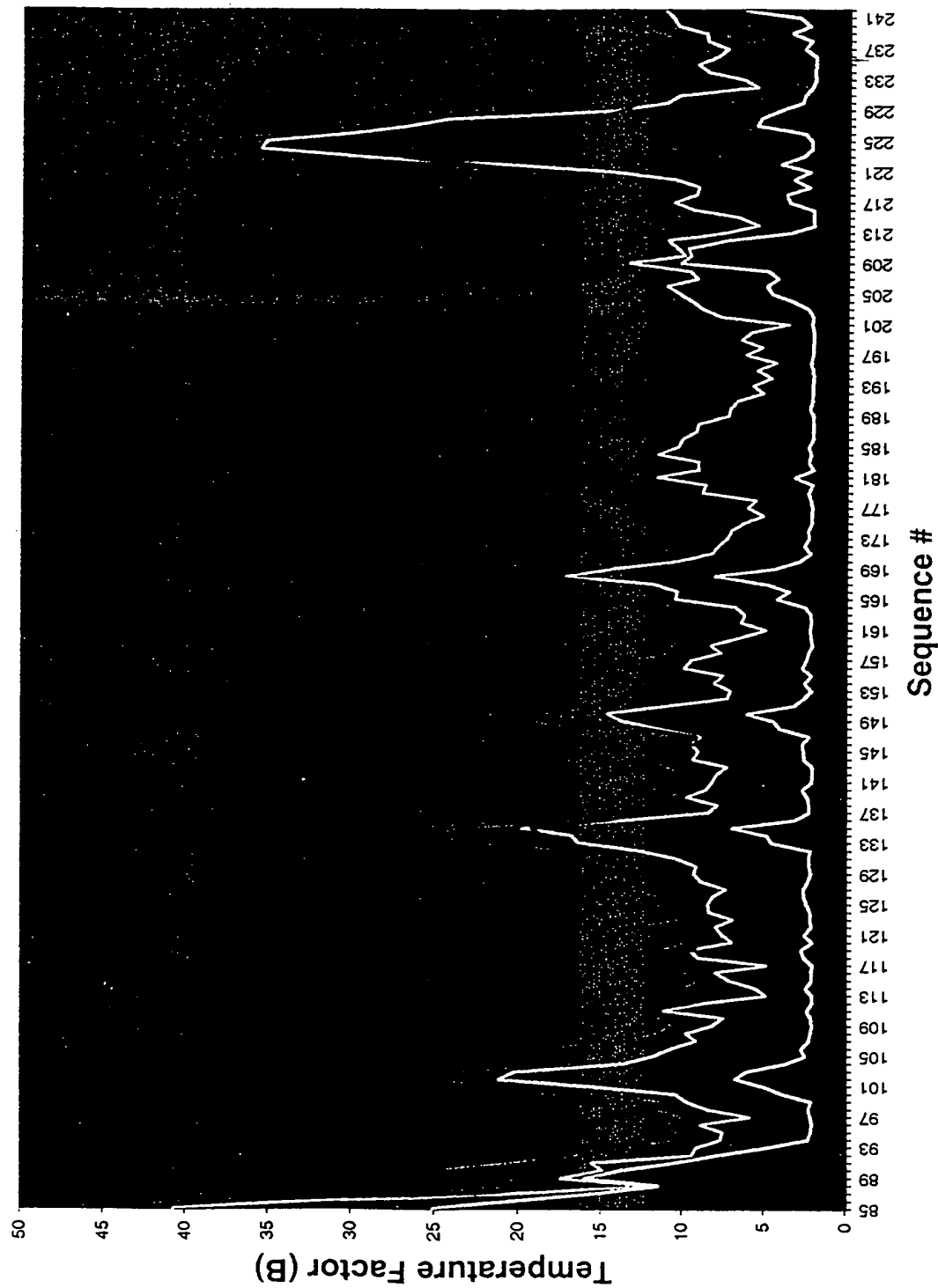
Figure 12



Superposition of Structures of MMP-8 Complexed with XII and XI

Figure 13

Temperature Factor Distribution of mmp-8 Complexes



XII (red)
IX (orange)
X (yellow)
XI (blue)
XIV (white)

Figure 14

(ϕ , ψ) Distribution Among the Residues from 222 to 231

	222 (R)	223 (E)	224 (T)	225 (S)	226 (N)					
I	-143.1	145.4	-50.0	128.2	-102.1	-14.3	-48.1	-31.1	-147.0	43.3
II	-132.7	133.2	-76.8	126.3	-112.1	134.8	-124.7	-16.2	-145.6	-174.7
III	-154.5	134.9	-73.5	145.4	-141.2	115.8	-89.0	-23.2	-136.0	-161.4
IV	-142.1	129.3	-74.5	134.3	-125.4	149.0	-128.8	-10.4	-144.1	-168.4
X1	-151.0	145.4	-48.5	130.0	-105.1	-10.5	-55.9	-29.2	-144.8	45.9
X2	-156.8	143.9	-43.9	129.5	-108.0	-9.7	-54.9	-29.8	-145.1	40.5

	227 (Y)	228 (S)	229 (L)	230 (P)	231 (Q)					
I	-66.4	137.6	-139.7	147.8	-48.4	124.5	-60.7	152.7	-46.1	-44.3
II	-91.6	28.1	-86.5	126.1	-96.1	149.1	-59.7	152.2	-54.4	-35.0
III	-99.2	28.6	-92.2	127.0	-90.6	149.7	-61.1	155.6	-55.0	-42.0
IV	-97.7	21.7	-85.3	128.3	-85.4	159.9	-62.8	156.6	-56.3	-40.1
X1	-74.2	143.6	-143.0	153.8	-54.7	138.0	-66.6	158.4	-46.3	-51.6
X2	-70.4	140.5	-138.9	157.2	-54.4	136.8	-67.6	157.8	-46.1	-50.5

Figure 15



Inhibitor XIV Binding Pocket

Figure 16



Inhibitor XI Binding Pocket